

CHB -604

- Wave –Particle Duality
- Wave equation
- Schrodinger wave equation-1-D
- Schrodinger wave equation-3-D
- Normalized and orthogonal wave function
- Acceptable wave functions- conditions

Introduction

De Broglie Hypothesis:

In quantum mechanics, any object can behave both like wave-particle duality at the sub-microscopic level.

Wave-particle Duality:

An object can act as both wave and particle at a same time. This phenomenon is called wave-particle duality.

So, the object would have energy packets, momentum(can be passed to another object), wave length, frequency and amplitude etc.

By using photo-electric effect and Compton effect we can easily describe about the wave particle duality

De Broglie (1924)

- Suggested that particles such as electrons might show wave properties.
- He summarised that the **de Broglie wavelength**, λ was given by:

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

m = mass

v = velocity of the particle

MATTER WAVES:

- de Broglie determined the wavelength of matter waves using the following equation:

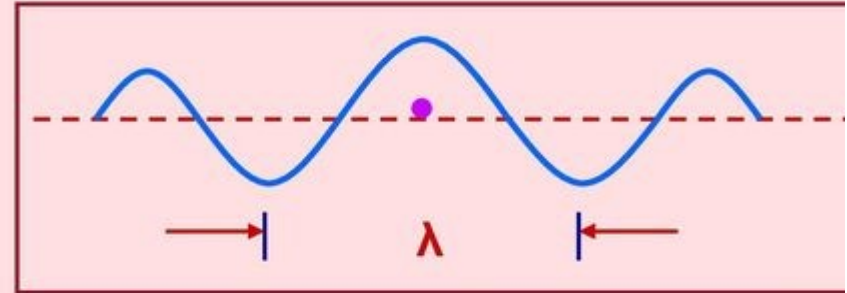
$$\lambda = \frac{h}{mv}$$

wavelength (of a matter wave)	λ	m (metres)
Planck's constant	h	J · s (joule seconds)
mass	m	kg (kilograms)
velocity	v	$\frac{\text{m}}{\text{s}}$ (metres per second)

de Broglie wave:

According to de Broglie, a moving material particle can be associated with a wave. i.e. a wave can guide the motion of the particle.

The waves associated with the moving material particles are known as de Broglie waves or matter waves.



Expression for de Broglie wave:

According to quantum theory, the energy of the photon is $E = h\nu = \frac{hc}{\lambda}$

According to Einstein's theory, the energy of the photon is $E = mc^2$

So, $\lambda = \frac{h}{mc}$ or $\lambda = \frac{h}{p}$ where $p = mc$ is momentum of a photon

If instead of a photon, we have a material particle of mass m moving with velocity v , then the equation becomes

$$\lambda = \frac{h}{mv}$$

which is the expression for de Broglie wavelength.

Einstein's equation , $E = mc^2$ (1)

Planck' equation, $E = hv$... (2)

Equating (1) and (2), we get $mc^2 = hv$..(3)

Since, $v = c / \lambda$,

therefore (3), $mc^2 = hc / \lambda$ or, $mc = h / \lambda$..(4)

or, $\lambda = h / mc$..(5)

For macroscopic objects , velocity 'v' can replace speed of light 'c'

Thus (5) becomes, $\lambda = h / mv$

Now, $mv = p$ (momentum of particle)

Therefore, $\lambda = h / p$

Wave Equation

Since electrons possess wave like properties, its motion may be described by a wave equation. Generally wave equation is represented mathematically by a second order differential equation.

Consider the wave motion of the vibration of stretched string.

If w be the amplitude of vibration at any point P whose coordinate is x at any instant of time t , then the differential equation for wave motion is given by

$$\frac{\partial^2 w}{\partial x^2} = \frac{1}{u^2} \frac{\partial^2 w}{\partial t^2} \quad \text{--- 1)}$$

where u = velocity of propagation of wave known as phase velocity
Equation may be solved by separating the variables

$$w = f(x), g(t) \quad \text{--- 2)}$$

where $f(x)$ is the function of coordinate x only and
 $g(t)$ " " " " time, t only

For a motion of standing wave such as occurs in a stretched string

$$g(t) = A \sin 2\pi \nu t \quad \text{--- 3)}$$

where ν = Frequency of vibration and A = Constant (Max. amplitude)

Equation 2) may be written as

$$w = f(x) \cdot A \sin 2\pi \nu t \quad \text{--- 4)}$$

$$\frac{\partial^2 w}{\partial t^2} = -f(x) 4\pi^2 \nu^2 A \sin 2\pi \nu t \quad \text{--- 5)}$$

$$\text{or, } \frac{\partial^2 w}{\partial t^2} = -4\pi^2 \nu^2 f(x) g(t) \quad \text{--- 6)}$$

$$\text{From eq}^n \text{ 2) } \frac{\partial^2 w}{\partial x^2} = \frac{\partial^2 f(x)}{\partial x^2} \cdot g(t) \quad \text{--- 7)}$$

$$\text{From eq}^n \text{ 1) and eq}^n \text{ 7), } \frac{\partial^2 f(x)}{\partial x^2} g(t) = \frac{1}{u^2} \frac{\partial^2 w}{\partial t^2} \quad \text{--- 7a)}$$

Using eqⁿ 6), $\frac{\partial^2 f(x)}{\partial x^2} \cdot g(t) = \frac{1}{u^2} (-4\pi^2 \nu^2 f(x) g(t))$
 $= -\frac{4\pi^2 \nu^2}{u^2} f(x) \quad \dots \dots \dots 8)$

\therefore the frequency of vibration ν and velocity u are related by eqⁿ

$$u = \nu \lambda \quad \text{or,} \quad u^2 = \lambda^2 \nu^2$$

Equation 8) becomes

$$\boxed{\frac{\partial^2 f(x)}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} f(x)} \quad \dots \dots \dots 9)$$

\checkmark Wave motion in 1-dimension

It may be extended in the 3-D represented by the coordinates x, y, z of $f(x)$, for one coordinate is replaced by $\Psi(x, y, z)$

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} = -\frac{4\pi^2}{\lambda^2} \Psi(x, y, z) \quad \dots \dots \dots 10)$$

or, $\boxed{\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} = -\frac{4\pi^2}{\lambda^2} \Psi} \quad \dots \dots \dots 11)$

\checkmark Wave equation for wave motion along 3-dimension x, y, z

Schrödinger Wave Equation

E. Schrödinger utilized the de Broglie's concept of matter wave and obtained wave equation for the material particles including electron.

Acc to de Broglie's relationship

$$\lambda = \frac{h}{p} \quad ; \quad \lambda^2 = \frac{h^2}{p^2} \quad \text{or} \quad \frac{1}{\lambda^2} = \frac{p^2}{h^2} \quad ; \quad p = \text{momentum} \quad ; \quad h = \text{Planck's const}$$

Putting the value of λ^2 in equation 11),

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} = -\frac{4\pi^2 p^2}{h^2} \Psi \quad \dots \dots \dots 12)$$

If $\Psi(x, y, z)$ is represented as ψ which is a function of position, is the potential energy of the particle and the kinetic energy is T